

Spin-orbit-coupling induced domain-wall resistance in diffusive ferromagnets

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Intrinsically disordered itinerant ferromagnetic alloys are not readily amenable to theoretical investigation because of their complexity. The study of disordered magnetic domain walls (DWs) is more difficult still because the magnetization direction changes gradually over long length scales. In this paper, we investigate diffusive transport through Permalloy DWs, taking into account non-collinearity, alloy disorder, and spin-orbit coupling fully quantum mechanically, from first principles. In addition to the effects of magnetization mistracking and anisotropic magnetoresistance, we find a new contribution to the resistance of a DW that comes from spin-orbit-coupling mediated spin-flip scattering in a textured diffusive ferromagnet.

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Introduction. Ferromagnetic alloys such as CoFeB or Permalloy (Py), $\text{Ni}_{80}\text{Fe}_{20}$, form the backbone of existing magnetoelectronic devices [1] such as spin valves and magnetic tunnel junctions [2]. They will play a central role in spin-transfer torque (STT) devices such as MRAMS (magnetic random-access memories) [3, 4], spin-torque oscillators (STOs) [5–7], and so-called “racetrack memories” [8, 9] based upon the “spin-transfer torque” (STT) effect whereby a spin-polarized current exerts a torque on a magnetization forcing it to precess [5, 10, 11]. A realistic description of electrical transport in itinerant ferromagnets is made difficult by the degeneracy of the partially filled d bands that are responsible for the magnetism and result in complicated Fermi surfaces for ordered materials. The concepts of Bloch states and Fermi surfaces that enable the development of transport theories for crystals are lost in disordered alloys. Even though the spin-orbit coupling (SOC) is in energy terms small, it has a large effect on the transport properties of magnetic alloys and must be included in any realistic description [12]. Finally, the STT effect results when electrical currents flow between materials whose magnetizations are not collinear; in the case of DWs, the length scales over which the magnetization changes is of order 10-100 nm [13]. These difficulties all stand in the way of a satisfactory description of transport properties of Py [14], currently the most important candidate for applications. We recently extended an efficient scattering formalism of spin transport [15] to include SOC that then successfully describes the transport properties of alloys such as Py [16]. In this Letter, we extend this to treat non-collinearity and report on an application to the resistance of Py DWs.

Most early theoretical studies of DW resistance (DWR) focussed on the effect of magnetization mistracking, the inability of conduction electrons to adiabatically follow an exchange potential rapidly varying in space that results in a positive DWR [17]; other mechanisms involving impurity scattering in DWs were found to decrease

the resistance [18, 19]. Much experimental effort has been made to identify whether the DWR is positive or negative [20–22] and, for the technologically important Py, both signs have been reported [23–25]. An additional complication presented by Py is the anisotropic magnetoresistance (AMR), a dependence of the resistivity on the angle between the current and magnetization directions that results from SOC. In the early theoretical models, SOC was neglected. Recent studies in ballistic metals or semiconductors show that SOC gives rise to an intrinsic DWR independent of the DW width because the number of allowed propagating channels only depends on the magnetization direction [26, 27]. In the diffusive regime, such a non-local effect is eliminated by disorder scattering and how SOC affects the DWR is still unclear.

The detailed electronic structure of itinerant ferromagnets makes an important contribution to DWR [28] and various approaches have been developed to study DWRs in particular materials from first-principles [29–32]. Our scattering approach takes the full electronic structure into account and allows us to treat alloy disorder, SOC and non-collinear magnetism on equal footings and study the resistance of Py DWs. A detailed analysis shows that three mechanisms contribute to the DWR of diffusive systems: magnetization mistracking results in an additional resistance inversely proportional to the DW width which is only observable in narrow DWs; AMR dominates the DWR of wide DWs if there is a component of the magnetization parallel to the current direction that changes through the DW; a new adiabatic DWR in diffusive DWs that results from SOC-mediated spin-flip scattering and is independent of the DW width and profile. It survives in the adiabatic limit and is able to distinguish an arbitrarily wide DW from the corresponding collinear ferromagnet.

Methods. To study electronic transport through a DW, we attach semiinfinite (copper) leads to a finite thickness of substitutional $\text{Ni}_{80}\text{Fe}_{20}$ alloy (Fig. 1) and

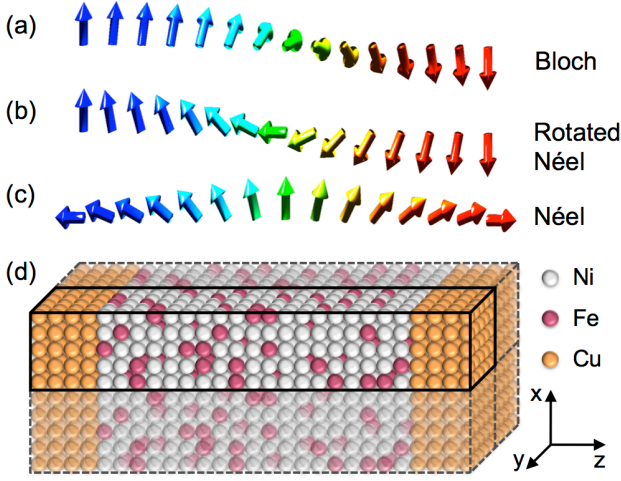


FIG. 1. (color online). Schematic illustration of the magnetic configurations of (a) Bloch, (b) rotated Néel, and (c) Néel DWs. (d) Sketch of the scattering geometry used in the calculations in which a finite thickness of Ni₈₀Fe₂₀ substitutional alloy is sandwiched between semiinfinite copper leads and alloy disorder is modelled using 5×5 lateral supercells periodically repeated in the *x-y* plane. Transport is in the *z* direction.

rotate the local magnetizations inside the scattering region to make a 180° DW. We considered three types of magnetization profiles, $\mathbf{m} = [m_x(z), m_y(z), m_z(z)]$, corresponding to Bloch $[-f(z), -g(z), 0]$, rotated Néel $[-f(z), 0, -g(z)]$, and Néel $[g(z), 0, f(z)]$ DWs. $g(z) = \text{sech}(\frac{z-r_W}{\lambda_W})$ and $f(z) = \tanh(\frac{z-r_W}{\lambda_W})$ for Walker (W) profiles while for linear (L) profiles, $f(z) = \sin \pi(\frac{z-r_L}{\lambda_L})$ and $g(z) = \cos \pi(\frac{z-r_L}{\lambda_L})$. Here $r_{W/L}$ is the DW center and $\lambda_{W/L}$ defines the width.

The electronic structure is first calculated self-consistently without SOC for a slab of collinear Py sandwiched between Cu leads using a surface Green's function method [33] implemented with a minimal basis of tight-binding linearized muffin-tin orbitals (TB-LMTOs) [34]. In the scattering region, potentials, charge- and spin-densities inside Ni and Fe atomic spheres (AS) are obtained using the coherent potential approximation. The local density approximation is employed with the exchange-correlation functional parameterized by von Barth and Hedin [35]. In the transport calculation, the self-consistent spin-up and spin-down AS potentials are distributed at random in a 5×5 lateral supercell subject to the 4:1 Ni-Fe concentration appropriate for Py and rotated in spin space as dictated by the DW profile. The whole scattering region with a length of 68 nm contains some 8300 atoms. The scattering matrix is calculated at the Fermi energy using a “wave-function matching” scheme [36] also implemented with TB-LMTOs [15] with SOC included [16]. The strength of the SOC, ξ_{SO} is determined from the potential gradient within atomic

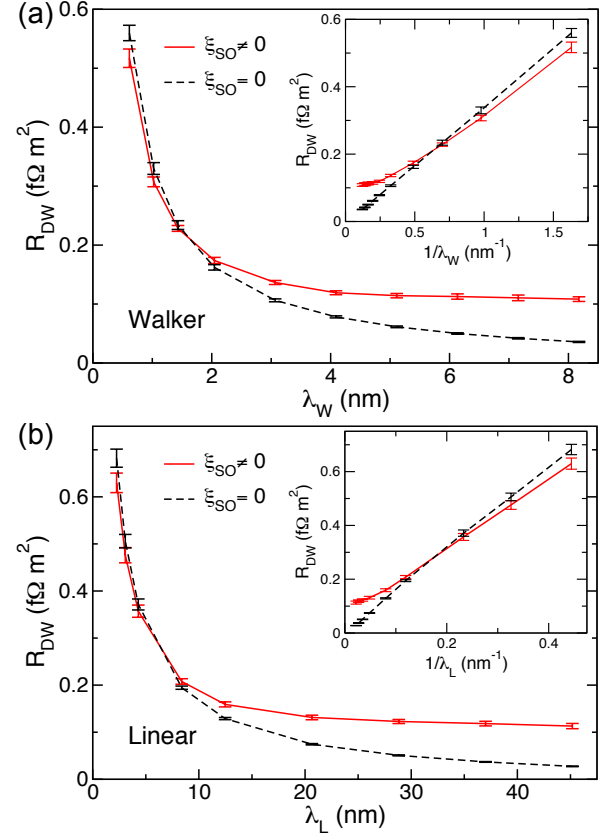


FIG. 2. (color online). DWR of Ni₈₀Fe₂₀ Bloch DWs with Walker (a) and Linear (b) profiles as a function of the respective width parameters. For each length, we typically consider 10 different disorder configurations and the error bars are a measure of the spread of the results. Insets: DWR replotted as a function of $1/\lambda_{W/L}$.

spheres. Within the Landauer-Büttiker formalism, we calculate the conductance of the system from the transmission matrix t as $G = (e^2/h)\text{Tr}(tt^\dagger)$. The DWR is defined as $R_{\text{DW}} = 1/G - 1/G_0$, where G_0 and G are the conductances of slabs of collinear Py and of a Py DW, respectively. G and G_0 are calculated with identical random atomic configurations and k -point sampling so as to exclude from R_{DW} spurious contributions from the Sharvin resistances of the leads and from the Cu|Py interfaces, and to focus on the resistance arising purely from the magnetization rotation.

Bloch DWs. The DWR is plotted as a function of the DW length in Fig. 2 for Bloch DWs whose magnetization rotates in a plane perpendicular to the transport direction so there is no contribution from the AMR. For a narrow DW, incident electrons see a rapidly varying (exchange) potential and are reflected by it giving rise to a large DWR that increases with decreasing DW width. This magnetization mistracking contribution decreases monotonically as the DW width increases and

vanishes in the wide-DW (adiabatic) limit in the absence of SOC (dashed lines). As shown in the insets, this contribution to the DWR is proportional to $1/\lambda$ for both Walker and linear DWs. The additional local resistivity due to the DW thus scales with $1/\lambda^2$ in agreement with earlier first-principles calculations [28] and theoretical models [17, 19]. It was also observed in a recent experiment [37] where the DW width in Pt|Co|Pt multilayer was tuned by ion beam irradiation.

SOC has very little effect on the DWR of narrow Bloch DWs which is dominated by mistracking. However, for long DWs, the DWR saturates to a finite value of about $0.1 \text{ f}\Omega\text{m}^2$ independent of whether the DW has a Walker or linear profile. We will refer to this SOC-related contribution that survives in the adiabatic limit and has not previously been identified as the adiabatic DWR, R_A . It distinguishes a DW from the corresponding collinear configuration and contradicts the universal assumption that conduction electrons follows a local magnetization adiabatically when they flow through a sufficiently wide DW.

The new contribution to the local resistivity is proportional to the magnetization gradient or $1/\lambda$ and can be understood by generalizing the Levy-Zhang model [17] as follows. In the presence of spin texture and SOC, the eigenstates are a mixture of spin-up $|\uparrow\rangle$ and spin-down $|\downarrow\rangle$ components based on the local quantization axis, i.e. $|\Psi_+\rangle = a|\uparrow\rangle + b|\downarrow\rangle$ and $|\Psi_-\rangle = -b^*|\uparrow\rangle + a^*|\downarrow\rangle$. If both spin texture and SOC are weak, $|a| \gg |b|$. A DW leads to a contribution to b that is, to leading order in perturbation theory, proportional to $1/\lambda$ [17]. In a relaxation time approximation, the contribution to the relaxation time from disorder scattering can be written in terms of a 2×2 local impurity potential v as

$$\begin{aligned} \frac{1}{\tau_{++}} &\propto \left| \langle \Psi_+ | \begin{pmatrix} v_{\uparrow\uparrow} & v_{\uparrow\downarrow} \\ v_{\downarrow\uparrow}^* & v_{\downarrow\downarrow} \end{pmatrix} | \Psi_+ \rangle \right|^2 \\ &= |a|^4 v_{\uparrow\uparrow}^2 + 4|a|^2 v_{\uparrow\uparrow} \text{Re}(a^* b v_{\uparrow\downarrow}) + O(|b|^2), \\ \frac{1}{\tau_{+-}} &\propto |a|^4 |v_{\uparrow\downarrow}|^2 + 2|a|^2 \text{Re}(a^* b v_{\uparrow\downarrow}) (v_{\downarrow\downarrow} - v_{\uparrow\uparrow}) + O(|b|^2), \\ \frac{1}{\tau_{--}} &\propto |a|^4 v_{\downarrow\downarrow}^2 - 4|a|^2 v_{\downarrow\downarrow} \text{Re}(a^* b v_{\uparrow\downarrow}) + O(|b|^2). \end{aligned} \quad (1)$$

In the absence of SOC, scattering is spin-conserving so $v_{\uparrow\downarrow} = 0$ and spin mixing only results from the non-collinear magnetization, $b \propto 1/\lambda$. As formulated by Levy and Zhang, a DW leads to an extra term in the resistivity proportional to $1/\lambda^2$ via spin-conserving scattering [17]. SOC makes spin-flip scattering possible, $v_{\uparrow\downarrow} \neq 0$, so the leading order correction to $1/\tau$ depends linearly on b . The $1/\lambda^2$ terms are of higher order and can be neglected. Thus the local resistivity in a Py DW has the form $\rho(\lambda) = \rho_0 + R_A/\lambda + O(1/\lambda^2)$ and results in a constant resistance R_A in the adiabatic limit.

To confirm this qualitative picture, we performed calculations for spin spirals with a fixed pitch, measured in

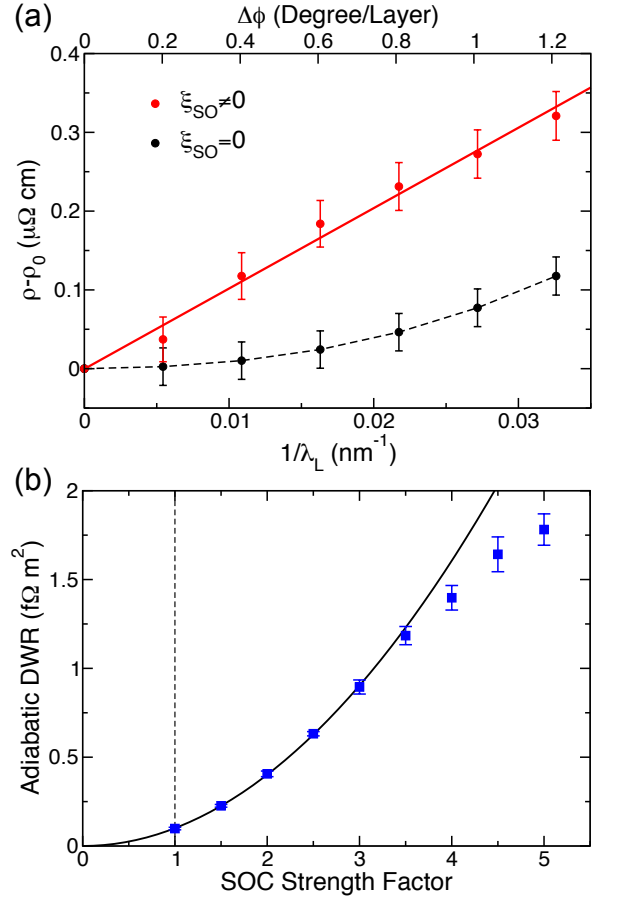


FIG. 3. (color online). (a) Difference between the resistivities of spin-spiral (ρ) and collinear (ρ_0) Py. The solid line is a linear fit to the data with SOC, yielding a slope $0.102 \pm 0.011 \text{ f}\Omega\text{m}^2$ in good agreement with the saturated DWR in Fig. 2. (b) Calculated saturation value of the DWR for Permalloy Walker Bloch DWs as a function of the SOC strength. The solid line shows a quadratic fitting. The vertical dashed line indicates the true SOC strength.

terms of the rotation $\Delta\phi$ of the magnetization between adjacent atomic layers, and varying the length of the spin spiral. The resistivity is then extracted from a linear fitting of the total resistance as a function of the length [16]. The difference in resistivities of spin-spiral (ρ) and collinear (ρ_0) Py is plotted in Fig. 3(a) as a function of $\Delta\phi$, or of the equivalent DW width $\lambda_L = \pi/\Delta\phi$. Without SOC, $\rho - \rho_0$ shows a quadratic dependence on $1/\lambda$ while the relation becomes linear in the presence of SOC. A linear fit (red solid line) yields the adiabatic DWR $R_A = 0.102 \pm 0.011 \text{ f}\Omega\text{m}^2$, that agrees well with the DWR calculations (Fig. 2).

From Eq. (1) it is not obvious how R_A will depend on ξ_{SO} because of the complicated interplay between the non-collinearity and SOC to affect b . To investigate this further, we increase ξ_{SO} artificially. Since the adiabatic DWR does not depend on the DW profile, we calculated

R_A for Walker Bloch DWs. As shown in Fig. 3(b), the adiabatic DWR rises monotonically with ξ_{SO} exhibiting a quadratic dependence up to a value 3.5 times the actual value. As the SOC in Py is quite small, this suggests that the adiabatic DWRs in materials containing heavy elements can be expected to be quite substantial.

Néel and rotated Néel DWs. Figure 4(a) shows the DWRs of Walker-profile Néel and rotated Néel DWs (solid lines) which contain a contribution from AMR. For sufficiently small values of λ_W , the DWR increases with decreasing DW width because of large magnetization mistracking and its behaviour is essentially independent of the DW type. For large values of λ_W , the DWR decreases for Néel walls and increases for rotated Néel walls essentially linearly as a function of λ_W . This behaviour can be understood in terms of the AMR. When the magnetization is parallel to the current direction, the resistivity ρ_{\parallel} of collinear Py is 20% larger than ρ_{\perp} , the value found when the magnetization is perpendicular to the current direction. In general, the local resistivity depends on the angle θ between magnetization and current as $\rho(\theta) = \rho_{\parallel} \cos^2 \theta + \rho_{\perp} \sin^2 \theta$ [12]. For wide DWs, we can estimate the contribution that the AMR makes to the DW resistance of Néel ($R_{\text{AMR}}^{\text{N}}$) and rotated Néel ($R_{\text{AMR}}^{\text{RN}}$) DWs as ($L \gg \lambda_W$)

$$R_{\text{AMR}}^{\text{N}} = \int_{r_W - \frac{L}{2}}^{r_W + \frac{L}{2}} dz \rho[\theta(z)] - \rho_{\parallel} L = -2\lambda_W(\rho_{\parallel} - \rho_{\perp}),$$

$$R_{\text{AMR}}^{\text{RN}} = \int_{r_W - \frac{L}{2}}^{r_W + \frac{L}{2}} dz \rho[\theta(z)] - \rho_{\perp} L = 2\lambda_W(\rho_{\parallel} - \rho_{\perp}). \quad (2)$$

The linear slopes at large λ_W in Fig. 4(a) agree with the analytical forms in Eq. (2). More quantitatively, we plot in Fig. 4(b) the difference between calculated DWRs of rotated Néel and Néel DWs as a function of λ_W (the solid symbols) and they are in perfect agreement with the analytical form $4\lambda_W(\rho_{\parallel} - \rho_{\perp})$ (the thick line), where $\rho_{\parallel(\perp)}$ are obtained from independent calculations for collinear Permalloy [16]. The linear width dependence suggests that the DWRs for wide Néel and rotated-Néel DWs are dominated by AMR. This picture is consistent with the experimentally observed transition from negative to positive DWR in Permalloy as the DW width is reduced to be atomically narrow [38]. If we subtract the AMR contribution from the total DWR using the analytical forms in Eq. (2), as shown by the dash-dotted lines in Fig. 4(a), we find the same width-dependence of DWRs as in Bloch DWs—the DWRs decrease with λ_W and saturate around $0.1 \text{ f}\Omega\text{m}^2$ corresponding to the adiabatic DWR.

Conclusions. A first-principles study of the resistance of Permalloy DWs underlines the importance of SOC. The total DWR in diffusive systems originates from magnetization mistracking, an adiabatic DWR, and AMR. In narrow DWs, magnetization mistracking leads to a large DWR that is independent of the DW type, is inversely

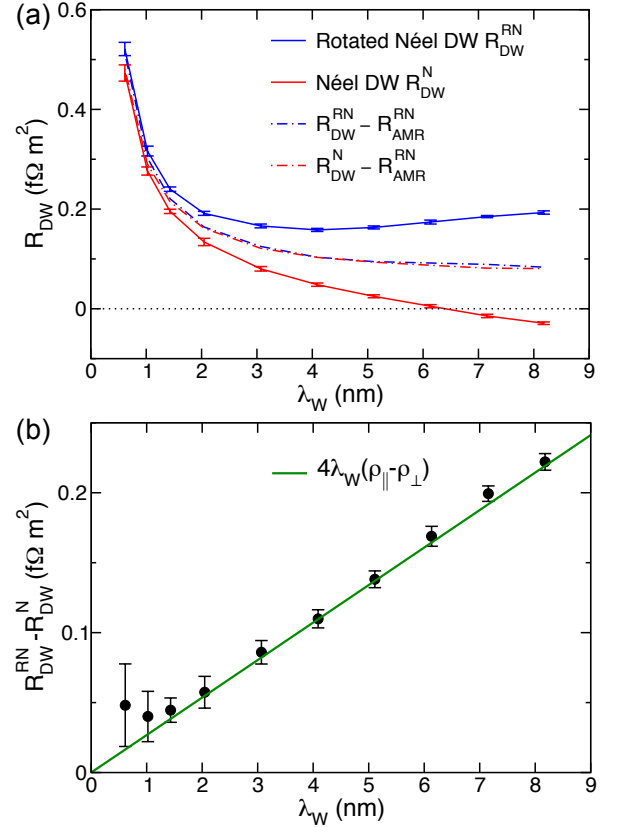


FIG. 4. (color online). (a) Calculated domain-wall resistance of $\text{Ni}_{80}\text{Fe}_{20}$ Néel and rotated Néel DWs with the Walker profile as a function of the width λ_W . The dash-dotted lines show the DWRs after subtracting the AMR contributions described by Eq. (2). (b) Difference between the DWRs for Néel and rotated Néel walls shown in (a). The thick line shows the analytical form $4\lambda_W(\rho_{\parallel} - \rho_{\perp})$ with $\rho_{\parallel(\perp)}$ taken from independent calculations for collinear Py [16].

proportional to the DW width and is dominated by spin-conserving scattering. The adiabatic DWR, which arises from the spin-flip scattering as a consequence of SOC, does not depend on the DW width. It implies a qualitative difference in the transport properties of a DW in the adiabatic limit and a collinear ferromagnet. In wide DWs, the DWR is dominated by AMR which is proportional to the DW width if there is a change in the angle between the current and local magnetization directions.

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